

# Junction between surfaces of two topological insulators

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We study the properties of a line junction which separates the surfaces of two three-dimensional topological insulators. The velocities of the Dirac electrons on the two surfaces may be unequal and may even have opposite signs. For a time reversal invariant system, we show that the line junction is characterized by an arbitrary parameter  $\alpha$  which determines the scattering from the junction. If the surface velocities have the same sign, we show that there can be edge states which propagate along the line junction with a velocity and orientation of the spin which depend on  $\alpha$  and the ratio of the velocities. Next, we study what happens if the two surfaces are at an angle  $\phi$  with respect to each other. We study the scattering and differential conductance through the line junction as functions of  $\phi$  and  $\alpha$ . We also find that there are edge states which propagate along the line junction with a velocity and spin orientation which depend on  $\phi$ . Finally, if the surface velocities have opposite signs, we find that the electrons must transmit into the two-dimensional interface separating the two topological insulators.

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## I. INTRODUCTION

Recent years have witnessed extensive theoretical<sup>1-7</sup> and experimental<sup>8-17</sup> studies of a class of two- and three-dimensional materials called topological insulators; for reviews, see Refs. 18 and 19. A topological insulator (TI) is a material which is gapped in the bulk but has gapless states at the surface which is one- or two-dimensional if the TI is two- or three-dimensional. Further, the electrons have strong spin-orbit coupling, and the surface states are described by a massless Dirac equation (in one or two dimensions) in which the directions of the spin angular momentum and linear momentum are tied to each other; they both lie in the plane of the surface and they are perpendicular to each other. The three-dimensional TIs come in two classes, strong and weak, which respectively have an odd and even number of massless Dirac cones at the surface<sup>2-4,6</sup>. In strong TIs, the gaplessness of an odd number of Dirac cones is protected by time reversal invariance; time reversal invariant perturbations such as non-magnetic disorder and lattice imperfections do not produce a gap, while time reversal breaking terms such as magnetic impurities or an external magnetic field can produce a gap for the surface states. For materials such as HgTe, Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>, specific surfaces have been found which have a single Dirac cone at one point of the two-dimensional Brillouin zone<sup>8,10,12,14-16</sup>. Several features of these surface Dirac electrons have been investigated recently. These include the existence of Majorana fermion modes at a magnet-superconductor interface<sup>20-23</sup>, anomalous magnetoresistance of ferromagnet-ferromagnet junctions<sup>24</sup>, realization of a switch by magnetically tuning the transport of the electrons by a proximate ferromagnetic film<sup>25</sup>, spin textures with chiral properties<sup>14-16</sup>, and the anisotropy of spin polarized scanning tunneling microscope (STM) tunneling into the surface of a TI<sup>26</sup>. Some general properties of the surface states and their scattering at the edges of two- and three-dimensional TIs have been studied in

Ref. 27.

A recent paper<sup>28</sup> has studied what happens when two three-dimensional TIs are brought close to each other so that their surfaces touch each other along a line; we will call this a line junction. This produces a system in which two two-dimensional surfaces governed by massless Dirac equations, with possibly different velocities  $v_1$  and  $v_2$ , share a one-dimensional boundary; similar studies have been carried out in Refs. 29 and 30 and in one dimension in Ref. 31. If a plane wave is incident on the boundary from one side with an angle of incidence  $\theta$ , it will be reflected and transmitted with certain amplitudes which depend on  $\theta$  and the ratio of velocities  $v_1/v_2$ . Ref. 28 made the interesting observation that if the velocities  $v_1$  and  $v_2$  have the same sign, the scattering problem can be solved in a straightforward way, but if they have opposite velocities, there is a difficulty; at least for the case of normal incidence, conservation of spin implies that the reflection and transmission amplitudes must both vanish. The way out of this difficulty is to consider two more sets of surface states which lie at the interface of the two TIs; then these states necessarily have some gapless states, even if one takes into account tunneling between them. Ref. 28 proposed that a low-energy plane wave which is incident normally on the line junction must get transmitted into these interface states.

In this paper, we will generalize the study of a junction between two TI surfaces in several ways. In Sec. II, we will consider the case of velocities with the same sign. We find that the most general condition at the line junction which conserves the current has one arbitrary parameter  $\alpha$  if we assume time reversal invariance. (The condition assumed in Ref. 28 corresponds to the special case of  $\alpha = 0$ ). We will compute the reflection and transmission amplitudes across the line junction as functions of  $\theta$ ,  $\alpha$  and the ratio of the velocities on the two sides of the line junction. We will also show that depending on the values of  $\alpha$  and the ratio of the two velocities, there can be edge states which travel along the line junction with a momen-

tum  $k$  but decay exponentially perpendicular to it. The velocity of the edge states along the junction is smaller than the velocities of the plane waves propagating far from the junction, while the spin orientation of the edge states has a component pointing out of the surface in contrast to the plane waves whose spins lie in the surface. In Sec. III, we will consider a TI which has two surfaces which meet at a line junction at an angle  $\phi$ ; we will show that this provides an interesting scattering problem in which the reflection and transmission amplitudes depend on  $\theta$ , the bending angle  $\phi$  and the parameter  $\alpha$ . We will use the transmission probability to compute the differential conductance across the line junction. Further, we will show that for  $\phi \neq 0$ , there are edge states which travel along the line junction with a momentum  $k$  but decay exponentially away from the junction; the velocity and the spin orientation of these states depend on  $\phi$ . In Sec. IV, we will examine the case of two TI surfaces where the velocities have opposite signs, and we will introduce an interface with two additional surfaces. We will explicitly derive the energy spectrum and wave functions at the interface assuming a simple form of the tunneling between the interface surfaces. We will then demonstrate that a wave incident on the surface indeed transmits into these states although the reflection and the transmission amplitudes on the surface are generally non-zero if the angle of incidence  $\theta \neq 0$ . In Sec. V, we will point out some ways by which the edge states moving along the junction may be experimentally detected, and we will make some concluding remarks. In the Appendix, we will study the most general boundary condition which is consistent with the Hermiticity of the Hamiltonian and the conservation of the current at the junction in the model discussed in Sec. II. We will show that the general condition involves four real parameters. However, if we assume that the system is invariant under time reversal, then there can be only one parameter; physically this corresponds to the strength of a potential barrier which may be present at the junction.

## II. JUNCTION BETWEEN SURFACE VELOCITIES WITH SAME SIGN

In this section, we will study a system with a line junction which separates the surfaces of two three-dimensional TIs, labeled 1 and 2. The surfaces define the  $x-y$  plane, and the line junction lies along  $y=0$ , as shown in Fig. 1; a thin barrier may be present along  $y=0$  as we will discuss below. The Hamiltonians in the two regions,  $y < 0$  and  $y > 0$ , are given by the two-dimensional massless Dirac form

$$\begin{aligned} H_1 &= -iv_1 (\sigma^x \partial_y - \sigma^y \partial_x), \\ H_2 &= -iv_2 (\sigma^x \partial_y - \sigma^y \partial_x), \end{aligned} \quad (1)$$

where  $\sigma^a$  denote Pauli matrices, and  $v_1, v_2$  denote the Fermi velocities on the two surfaces respectively. We will assume here that  $v_1, v_2 > 0$ . The Hamiltonians  $H_i$  in

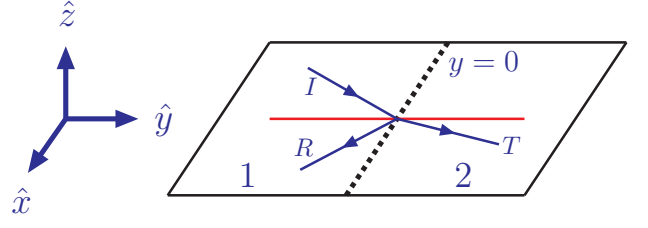


FIG. 1: (Color online) Schematic picture of two regions of the  $x-y$  plane, labeled 1 and 2, which are separated by a line junction at  $y=0$  where a thin barrier may be present. A wave incident ( $I$ ) from region 1 and the corresponding reflected ( $R$ ) and transmitted ( $T$ ) waves are shown.

Eq. (1) act on wave functions  $\psi_i$ , where  $i=1$  and  $2$  for  $y < 0$  and  $y > 0$ , respectively. (We will generally set  $\hbar = 1$  everywhere.)

Hamiltonians defined in disjoint regions, such as the ones given in Eq. (1), do not define a system completely; this has been emphasized earlier for the Dirac equation in one dimension<sup>31</sup>. To define the system fully, we need to specify the boundary conditions that the wave functions must satisfy at  $y=0$  in order to ensure that the Hamiltonian  $H$  of the entire system, given by  $H_1$  for  $y < 0$  and  $H_2$  for  $y > 0$ , is Hermitian, namely, that

$$\begin{aligned} & \int_{-\infty}^{\infty} dx \left[ \int_{-\infty}^{0-} dy + \int_{0+}^{\infty} dy \right] \chi'^{\dagger} H \chi \\ &= \int_{-\infty}^{\infty} dx \left[ \int_{-\infty}^{0-} dy + \int_{0+}^{\infty} dy \right] (H \chi')^{\dagger} \chi \end{aligned} \quad (2)$$

for any two wave functions  $\chi$  and  $\chi'$  which satisfy the boundary conditions. On doing an integration by parts with  $\partial_y$ , we find that Eq. (2) requires

$$v_1 ((\chi_1')^{\dagger} \sigma^x \chi_1)_{y \rightarrow 0-} = v_2 ((\chi_2')^{\dagger} \sigma^x \chi_2)_{y \rightarrow 0+}. \quad (3)$$

We may now ask: what is the most general linear relation between  $(\chi_1)_{y \rightarrow 0-}$  ( $(\chi_1')_{y \rightarrow 0-}$ ) and  $(\chi_2)_{y \rightarrow 0+}$  ( $(\chi_2')_{y \rightarrow 0+}$ ) which satisfies Eq. (3)? The answer to this is discussed in detail in the Appendix; we show there that the general linear relation involves four arbitrary real parameters, and we provide a physical understanding of these parameters. We then argue that if the system is invariant under time reversal, the linear relation involves only one real parameter  $\alpha$  and is given by

$$(\chi_2)_{y \rightarrow 0+} = \sqrt{\frac{v_1}{v_2}} e^{-i\alpha\sigma^x} (\chi_1)_{y \rightarrow 0-}, \quad (4)$$

and similarly between  $(\chi_2')_{y \rightarrow 0+}$  and  $(\chi_1')_{y \rightarrow 0-}$ . We note that changing  $\alpha \rightarrow \alpha + \pi$  has no effect on any physical quantities (such as reflection and transmission probabilities) since this is just equivalent to changing  $\psi_2 \rightarrow -\psi_2$ . In the rest of this paper, we will assume that  $\alpha$  lies in the

range  $-\pi/2 \leq \alpha \leq \pi/2$ . In Refs. 28–31, the relation between the wave functions at the line junction was taken to be

$$(\chi_2)_{y \rightarrow 0+} = \sqrt{\frac{v_1}{v_2}} (\chi_1)_{y \rightarrow 0-}. \quad (5)$$

Clearly this is a special case of Eq. (4) corresponding to  $\alpha = 0$ .

Given the form of the Hamiltonians in Eq. (1), the current density  $\vec{J}_i = (J_{ix}, J_{iy})$  on surface  $i$  ( $= 1, 2$ ) is given by

$$\vec{J}_i = v_i (-\psi_i^\dagger \sigma^y \psi_i, \psi_i^\dagger \sigma^x \psi_i). \quad (6)$$

[This can be derived by using the equation of motion  $i\partial_t \psi_i = H_i \psi_i$  and the equation of continuity  $\partial_t \rho_i + \vec{\nabla} \cdot \vec{J}_i = 0$ , where the charge density is  $\rho_i = \psi_i^\dagger \psi_i$ .] Current conservation in the  $\hat{y}$  direction at the line junction at  $y = 0$  implies that

$$v_1 (\psi_1^\dagger \sigma^x \psi_1)_{y \rightarrow 0-} = v_2 (\psi_2^\dagger \sigma^x \psi_2)_{y \rightarrow 0+}, \quad (7)$$

We now see that this is ensured by the same condition (4) which ensures Hermiticity of the Hamiltonian  $H$ .

The system described by Eqs. (1) and (4) is invariant under two discrete symmetries, namely, parity and time reversal. Under parity,  $x \rightarrow -x$  and  $\psi \rightarrow \sigma^x \psi$ . Under time reversal,  $t \rightarrow -t$  and  $\psi \rightarrow \sigma^y \psi^*$ .

### A. Scattering

For an electron far from the line junction, the eigenstates of the Hamiltonian are plane waves labeled by a momentum  $\vec{k} = (k_x, k_y)$ . For a velocity  $v_i > 0$ , the energy spectrum and wave functions are given by

$$\begin{aligned} \psi_+ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i\theta} \end{pmatrix} e^{i(k_x x + k_y y - E_+ t)}, \\ \psi_- &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{-i\theta} \end{pmatrix} e^{i(k_x x + k_y y - E_- t)}, \end{aligned} \quad (8)$$

for  $E_+ = v_i k$  and  $E_- = -v_i k$  respectively, where  $\cos \theta = k_y/k$ ,  $\sin \theta = k_x/k$ , and  $k = \sqrt{k_x^2 + k_y^2}$ . Note that the directions of the spin and momentum are tied to each other; for positive energy states, they are related by  $\vec{\sigma} = \vec{k} \times \hat{z}$ , where  $\hat{x}$ ,  $\hat{y}$  and  $\hat{z}$  form a right-handed coordinate frame.

Now let a plane wave be incident on the line junction from the left ( $y < 0$ ) with momentum  $\vec{k}_I = (k_{Ix}, k_{Iy})$  and positive energy  $E_+ = v_1 |\vec{k}_I|$ . The reflected and transmitted waves will have momenta  $\vec{k}_R = (k_{Rx}, k_{Ry})$  and  $\vec{k}_T = (k_{Tx}, k_{Ty})$  and amplitudes  $r$  and  $t$  respectively. We can determine all these quantities in terms of the incident momentum  $\vec{k}_I$  using conservation of energy, momentum in the  $\hat{x}$  direction (due to translation invariance in that

direction), and current conservation in the  $\hat{y}$  direction at the line junction. Conservation of energy implies that  $v_1 \sqrt{k_{Ix}^2 + k_{Iy}^2} = v_1 \sqrt{k_{Rx}^2 + k_{Ry}^2} = v_2 \sqrt{k_{Tx}^2 + k_{Ty}^2}$ , while conservation of momentum in the  $\hat{x}$  direction implies that

$$k_{Ix} = k_{Rx} = k_{Tx}. \quad (9)$$

These equations imply that

$$\begin{aligned} k_{Ry} &= -k_{Iy}, \\ k_{Ty} &= \frac{1}{v_2} \sqrt{v_1^2 (k_{Ix}^2 + k_{Iy}^2) - v_2^2 k_{Ix}^2}, \end{aligned} \quad (10)$$

assuming that the quantity inside the square root in the second equation is positive; otherwise  $k_{Ty}$  will be imaginary and we will have total internal reflection on the left side of the line junction<sup>28</sup>. Thus  $\vec{k}_R$  and  $\vec{k}_T$  are fixed in terms of  $\vec{k}_I$ . If we define  $\theta = \tan^{-1}(k_{Ix}/k_{Iy})$  and  $\theta' = \tan^{-1}(k_{Tx}/k_{Ty})$ , where  $-\pi/2 \leq \theta, \theta' \leq \pi/2$ , we have

$$\frac{1}{v_1} \sin \theta = \frac{1}{v_2} \sin \theta'. \quad (11)$$

Finally, current conservation in the  $\hat{y}$  direction at the line junction at  $y = 0$  implies that

$$v_1 k_{Iy} (1 - |r|^2) = v_2 k_{Ty} |t|^2. \quad (12)$$

The reflection and transmission amplitudes  $r$  and  $t$  can be obtained for the general boundary condition in Eq. (4). The general expressions for  $r$  and  $t$  are

$$\begin{aligned} t &= \sqrt{\frac{v_1}{v_2}} \frac{\cos \theta e^{i(\theta' - \theta)/2}}{\cos \alpha \cos(\frac{\theta + \theta'}{2}) + i \sin \alpha \cos(\frac{\theta - \theta'}{2})}, \\ r &= e^{-i\theta} \frac{\sin \alpha \sin(\frac{\theta + \theta'}{2}) + i \cos \alpha \sin(\frac{\theta' - \theta}{2})}{\cos \alpha \cos(\frac{\theta + \theta'}{2}) + i \sin \alpha \cos(\frac{\theta - \theta'}{2})}. \end{aligned} \quad (13)$$

For equal velocities  $v_1 = v_2$ , we have  $\theta' = \theta$  and Eq. (13) simplifies to

$$\begin{aligned} t &= \frac{\cos \theta}{\cos \alpha \cos \theta + i \sin \alpha}, \\ r &= \frac{e^{-i\theta} \sin \alpha \sin \theta}{\cos \alpha \cos \theta + i \sin \alpha}. \end{aligned} \quad (14)$$

Given the transmission amplitude  $t$ , we can compute the conductance across the line junction. This will be discussed in Sec. IV for a more general model in which the surfaces 1 and 2 are at an angle with respect to each other.

### B. Edge states

It turns out that for certain ranges of values of  $v_1/v_2$  and  $\alpha$ , there are edge states which propagate along the line junction (i.e., along the  $\hat{x}$  direction) with a momentum  $k$  and whose wave functions decay exponentially as

$y \rightarrow \pm\infty$ . At the line junction, let us look for unnormalized wave functions of the form

$$\begin{aligned}\psi_1 &= \begin{pmatrix} 1 \\ \gamma_1 \end{pmatrix} e^{i(kx-Et)+\chi_1 y} \text{ in region 1,} \\ \psi_2 &= \begin{pmatrix} \gamma_2 \\ \gamma_3 \end{pmatrix} e^{i(kx-Et)-\chi_2 y} \text{ in region 2,}\end{aligned}\quad (15)$$

where  $\gamma_1, \gamma_2, \gamma_3$  can be complex numbers but the  $\chi_i$  must be real and positive. The energy is given by  $E = \pm v_1 \sqrt{k^2 - \chi_1^2} = \pm v_2 \sqrt{k^2 - \chi_2^2}$ ; we must have  $\chi_1, \chi_2 \leq |k|$ . We now demand that the wave functions in Eq. (15) be eigenstates of Eq. (1) and that they satisfy Eq. (4); this gives us the values of the  $\gamma_i$  and  $\chi_i$ . Let us parametrize  $\chi_1/k = \sin \theta_1$  and  $\chi_2/k = \sin \theta_2$ , where  $-\pi/2 < \theta_1, \theta_2 < \pi/2$ . We further assume that  $v_1 \leq v_2$ , and define  $\beta = \cos^{-1}(v_1/v_2)$ , where  $0 \leq \beta < \pi/2$ . We then find that edge states exist under the following conditions. For  $\beta/2 < \alpha < \pi/2$ , the energy is negative and given by  $E = -v_1 \sqrt{k^2 - \chi_1^2}$ , while for  $-\pi/2 < \alpha < -\beta/2$ , the energy is positive and given by  $E = v_1 \sqrt{k^2 - \chi_1^2}$ . In both cases, the magnitude of the velocity,  $|E/k|$ , is given by

$$v = \frac{v_1 v_2 |\sin(2\alpha)|}{\sqrt{v_1^2 + v_2^2 - 2v_1 v_2 \cos(2\alpha)}}. \quad (16)$$

Further,

$$\begin{aligned}\tan \theta_1 &= -\text{sgn}(E/k) \frac{v_1 - v_2 \cos(2\alpha)}{v_2 \sin(2\alpha)}, \\ \tan \theta_2 &= -\text{sgn}(E/k) \frac{v_2 - v_1 \cos(2\alpha)}{v_1 \sin(2\alpha)}.\end{aligned}\quad (17)$$

where  $\text{sgn}$  denotes the signum function:  $\text{sgn}(z) \equiv +1$  if  $z > 0$  and  $-1$  if  $z < 0$ . Note that there are no edge states if  $-\beta/2 \leq \alpha \leq \beta/2$ .

We can use the above expressions to show that the velocity  $v$  is smaller than both  $v_1$  and  $v_2$ . To state this differently, for a given value of the  $\hat{x}$ -momentum  $k$ , the energy of the edge states has a smaller magnitude than the energy of the plane waves in both regions 1 and 2. (At the two points  $\alpha = \pm\beta/2$ , we find that  $v = v_1$ ).

The various expressions above simplify if  $v_1 = v_2$ . Then there are edge states in the entire range  $-\pi/2 < \alpha < \pi/2$ , with  $v = v_2 |\sin \alpha|$  and  $\theta_1 = \theta_2 = -\text{sgn}(E/k) \alpha$ . In Fig. 2, we present a plot of the velocity of the edge states as a function of  $\alpha$ , in the range  $-\pi/2 \leq \alpha \leq \pi/2$ , for  $v_1/v_2 = 1$  and 0.5.

We emphasize that the sign of the energy  $E$  of the edge states depends only on the sign of  $\alpha$ , and not on the sign of the momentum  $k$ . This is consistent with the time reversal invariance of the system; under time reversal, the momentum reverses sign but the energy remains the same.

After obtaining the values of the  $\gamma_i$  in Eq. (15), we can find the orientation of the spin of the edge states. For a spin-1/2 particle whose spin points along a unit

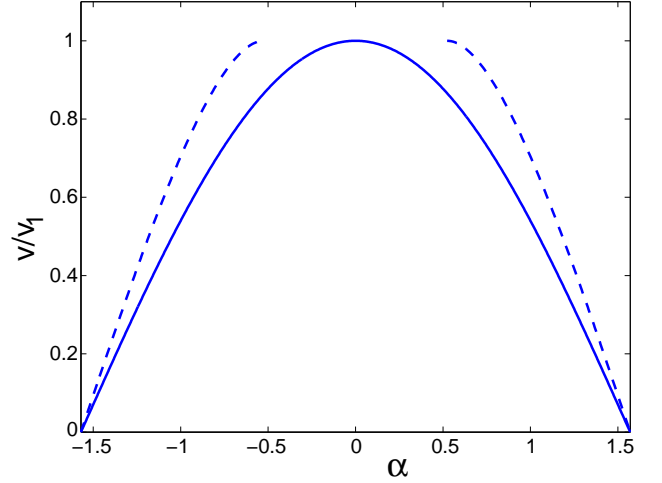


FIG. 2: (Color online) Plot of  $v/v_1$  versus  $\alpha$  for  $v_1/v_2 = 1$  (solid) and 0.5 (dashed).

vector  $\hat{n} = (\sin a \cos b, \sin a \sin b, \cos a)$ , we know that the normalized wave function is given by the transpose of  $(\cos(a/2), \sin(a/2)e^{ib})$ . Using this we find that the spin of the edge states points along the direction  $-\sin \theta_1 \hat{z} \mp \cos \theta_1 \hat{y}$  in region 1 and along the direction  $\sin \theta_2 \hat{z} \mp \cos \theta_2 \hat{y}$  in region 2, where the  $\mp$  signs refer to  $E > 0$  and  $< 0$  respectively. Thus the spin of the edge states lies in the  $y - z$  plane and *not* in the  $x - y$  plane which is the surface of the TIs.

To conclude this section, we see that several properties of the edge states depend only on the dimensionless parameters  $\alpha$  and  $v_1/v_2$ . This is true of the velocity  $E/k$ , the spin orientations in the two regions, and the product of  $k$  and the exponential decay lengths  $1/\chi_1$  and  $1/\chi_2$ .

### III. JUNCTION BETWEEN SURFACES AT AN ANGLE

We will now study what happens when there is a line junction between two surfaces which are boundaries of the same TI, but the surfaces are at an angle  $\phi$  with respect to each other; this is shown in Fig. 3. This is a realistic situation since any finite-sized TI must be bounded by surfaces meeting along lines. We will assume that the velocity  $v$  is the same and is positive on both surfaces. Region 1 forms the  $x - y$  plane, while region 2 forms the  $x - y'$  plane where  $\hat{y}' = \cos \phi \hat{y} - \sin \phi \hat{z}$ . In regions 1 and 2,  $y < 0$  and  $y' > 0$  respectively; the line junction lies at  $y = y' = 0$ , and we will again allow for a thin barrier to be present there. The Hamiltonians in the two regions are given by

$$\begin{aligned}H_1 &= -iv (\sigma^x \partial_y - \sigma^y \partial_x), \\ H_2 &= -iv (\sigma^x \partial_{y'} - \sigma^{y'} \partial_x),\end{aligned}\quad (18)$$

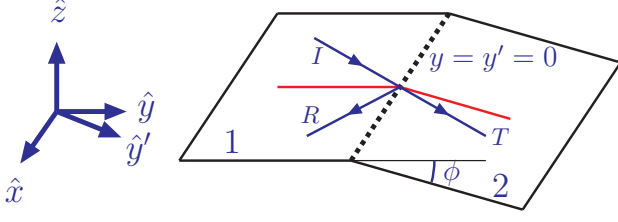


FIG. 3: (Color online) Schematic picture of two regions, labeled 1 and 2, separated by a line junction at  $y = y' = 0$  where a thin barrier may be present; the unit vectors normal to the two regions are at an angle  $\phi$  with respect to each other. A wave incident ( $I$ ) from region 1 and reflected ( $R$ ) and transmitted ( $T$ ) waves are shown.

where  $\sigma^{y'} = \cos \phi \sigma^y - \sin \phi \sigma^z$ . This model is of physical interest since any three-dimensional TI of finite size must necessarily have surfaces meeting along lines; our model describes the region around one such line. We will take  $\phi$  to lie in the range  $-\pi < \phi < \pi$ , although real systems may only allow a more restricted range of  $\phi$ . The system described in Eq. (18) is invariant under the parity and time reversal transformations.

We may now ask what the general linear condition must be between  $(\psi_1)_{y \rightarrow 0-}$  and  $(\psi_2)_{y' \rightarrow 0+}$  so that the Hamiltonian of the complete system is Hermitian. Following an analysis similar to the one given in the Appendix for the model in Sec. II, we find that the general relation involves four parameters. But if we demand that the system be invariant under time reversal, we find that the only one parameter can appear, namely,  $(\psi_2)_{y' \rightarrow 0+} = e^{-i\alpha\sigma^x}(\psi_1)_{y \rightarrow 0-}$ . This also ensures current conservation at the line junction, namely,

$$(\psi_1^\dagger \sigma^x \psi_1)_{y \rightarrow 0-} = (\psi_2^\dagger \sigma^x \psi_2)_{y' \rightarrow 0+}. \quad (19)$$

### A. Scattering

For plane waves, the energy spectrum and wave functions in region 1 have the form given in Eq. (8), while in region 2, we obtain

$$\begin{aligned} \psi_+ &= \frac{e^{-i\theta}}{\sqrt{2}} \begin{pmatrix} \cos \theta + i \sin \theta \cos \phi \\ 1 - \sin \theta \sin \phi \end{pmatrix} e^{i(k_x x + k_y y' - E_+ t)}, \\ \psi_- &= \frac{e^{-i\theta}}{\sqrt{2}} \begin{pmatrix} \cos \theta + i \sin \theta \cos \phi \\ -1 - \sin \theta \sin \phi \end{pmatrix} e^{i(k_x x + k_y y' - E_- t)}, \end{aligned} \quad (20)$$

where  $E_{\pm} = \pm v \sqrt{k_x^2 + k_y^2}$  and  $\theta = \tan^{-1}(k_x/k_y)$ . With the normalization given in Eq. (20), the currents in the  $y'$  direction are given by  $\psi_+^\dagger \sigma^x \psi_+ = \cos \theta (1 - \sin \theta \sin \phi)$  and  $\psi_-^\dagger \sigma^x \psi_- = -\cos \theta (1 + \sin \theta \sin \phi)$ .

We can then solve a scattering problem in which a wave is incident on the line junction from region 1 with momentum  $\vec{k}_I = (k_{Ix}, k_{Iy})$ , and gets reflected and transmitted with amplitudes  $r$  and  $t$  respectively. These amplitudes depend on the incident angle  $\theta$ , the bending angle  $\phi$ , and the parameter  $\alpha$ . The general expression for  $t$  is

$$\begin{aligned} t &= \frac{2 \cos \theta}{A_1 \cos \alpha + i A_2 \sin \alpha}, \\ A_1 &= \cos \theta + i \sin \theta \cos \phi + e^{-i\theta} (1 - \sin \theta \sin \phi), \\ A_2 &= 1 - \sin \theta \sin \phi + e^{-i\theta} (\cos \theta + i \sin \theta \cos \phi). \end{aligned} \quad (21)$$

We note that the transmission probability  $|t|^2$  remains the same if we simultaneously change  $\theta \rightarrow -\theta$ ,  $\alpha \rightarrow -\alpha$  and  $\phi \rightarrow -\phi$ . As a result, the conductance (to be discussed in the next section) remains the same if we simultaneously change  $\alpha \rightarrow -\alpha$  and  $\phi \rightarrow -\phi$ , but generally changes if  $\alpha \rightarrow -\alpha$  or  $\phi \rightarrow -\phi$  separately.

### B. Conductance

We will now compute the conductance across the line junction. Suppose that the system is coupled at the far left ( $y \rightarrow -\infty$ ) and far right ( $y' \rightarrow \infty$ ) to reservoirs with chemical potentials  $\mu_L$  and  $\mu_R$  respectively; we will assume that the reservoirs are at zero temperature. Electrons coming from one reservoir transmit across the line junction and go to the other reservoir with a probability given by  $|t|^2$  given in Eq. (21). Assuming that the system has a large width in the  $\hat{x}$  direction given by  $W$ , the net current going from left to right is given by

$$I = eW \int \int \frac{dk_x dk_y}{(2\pi)^2} |t|^2 v \cos \theta (1 - \sin \theta \sin \phi), \quad (22)$$

where  $e$  is the charge of an electron, and the factor of  $v \cos \theta (1 - \sin \theta \sin \phi)$  appears because we are interested in the  $y'$  component of the transmitted current in region 2. For the integral in Eq. (22), the energy  $E = \hbar v \sqrt{k_x^2 + k_y^2}$  goes from  $\mu_R$  to  $\mu_L$ , assuming that  $\mu_R < \mu_L$ , and the angle  $\theta = \tan^{-1}(k_x/k_y)$  goes from  $-\pi/2$  to  $\pi/2$ . The voltage applied to a reservoir is related to its chemical potential as  $\mu = qV$ ; in the zero bias limit,  $\mu_L, \mu_R \rightarrow \mu$ , we obtain the differential conductance

$$G = \frac{dI}{dV} = \frac{e^2 W \mu}{v(2\pi\hbar)^2} \int_{-\pi/2}^{\pi/2} d\theta |t|^2 \cos \theta (1 - \sin \theta \sin \phi). \quad (23)$$

Using Eqs. (21) and (23), we can calculate  $G$  as a function of  $\alpha$  and  $\phi$ . For  $\alpha = \phi = 0$ , we have  $t = 1$  and we obtain the conductance  $G_0 = 2e^2 W \mu / (v(2\pi\hbar)^2)$ .

Fig. 4 shows a plot of the conductance (in units of  $G_0$ ) as a function of  $\alpha$ , in the range  $-\pi/2 \leq \alpha \leq \pi/2$ , for  $\phi = 0$  (solid) and  $\pi/2$  (dashed). Fig. 5 shows a plot of the conductance as a function of  $\phi$ , in the range  $-\pi/2 \leq \phi \leq \pi/2$ , for  $\alpha = 0, \pi/4$  and  $\pi/2$ . Interestingly, we find that the conductance is unity (in units of  $G_0$ ) on the line  $\alpha = -\phi/2$ , where  $-\pi/2 \leq \alpha \leq \pi/2$ .

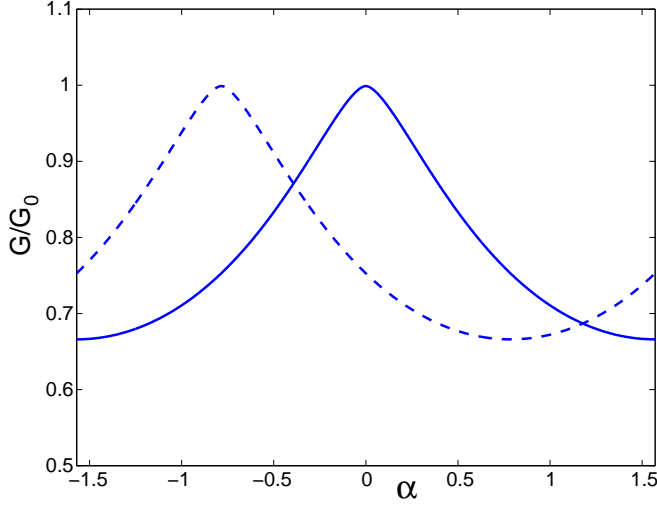


FIG. 4: (Color online) Plot of  $G/G_0$  versus  $\alpha$  for  $\phi = 0$  (solid) and  $\pi/2$  (dashed).

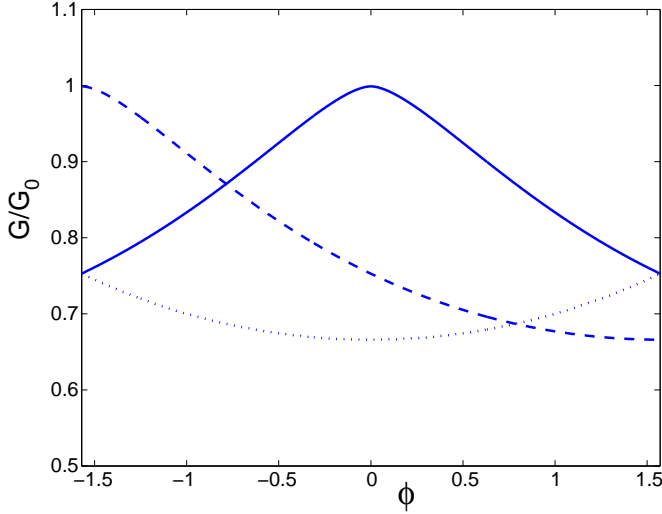


FIG. 5: (Color online) Plot of  $G/G_0$  versus  $\phi$  for  $\alpha = 0$  (solid),  $\pi/4$  (dashed) and  $\pi/2$  (dotted).

### C. Edge states

For any non-zero value of  $\phi$ , we find that there are edge states which propagate along the line junction with a momentum  $k$  and whose wave functions decay exponentially as either  $y \rightarrow -\infty$  or  $y' \rightarrow \infty$ . Let us set  $\alpha = 0$ , so that we have the boundary condition  $(\psi_2)_{y' \rightarrow 0+} = (\psi_1)_{y \rightarrow 0-}$  at the line junction. We now look for unnormalized wave functions of the form

$$\begin{aligned} \psi_1 &= \begin{pmatrix} 1 \\ \gamma \end{pmatrix} e^{i(kx - Et) + \chi y} \quad \text{in region 1,} \\ \psi_2 &= \begin{pmatrix} 1 \\ \gamma \end{pmatrix} e^{i(kx - Et) - \chi y'} \quad \text{in region 2,} \end{aligned} \quad (24)$$

where  $\gamma$  can be complex but  $\chi$  must be real and positive; the above wave functions satisfy the boundary condition given above. Demanding that these wave functions be eigenstates of Eq. (18), we find that there is an edge state for any non-zero values of  $k$  and  $\phi$ . Since  $-\pi < \phi < \pi$  and  $\phi \neq 0$ , we can use the facts that  $\cos(\phi/2)$  is always positive and that  $\sin(\phi/2)$  and  $\phi$  have the same sign. We then find that if  $\phi > 0$ , the edge state energy is negative and given by  $E = -v\sqrt{k^2 - \chi^2}$ , while if  $\phi < 0$ , the energy is positive and given by  $E = v\sqrt{k^2 - \chi^2}$ . In either case, we obtain the relation

$$\frac{\sqrt{k^2 - \chi^2}}{k - \chi} = \frac{\sqrt{k^2 - \chi^2} + k|\sin \phi|}{k \cos \phi + \chi}, \quad (25)$$

whose solution is given by

$$\chi = |k \sin(\phi/2)|. \quad (26)$$

For instance,  $\chi = |k\phi/2|$  for  $\phi \rightarrow 0$  and  $= |k|/\sqrt{2}$  for  $\phi = \pm\pi/2$ . The quantity  $\gamma$  in Eq. (24) is given by

$$\gamma = i \frac{\cos(\phi/2)}{\text{sgn}(k\phi) - \sin(\phi/2)}. \quad (27)$$

We conclude that several properties of the edge states depend only on the bending angle  $\phi$  and on the sign of the momentum  $k$ . The product of the exponential decay length  $1/\chi$  and  $|k|$  is equal to  $1/|\sin(\phi/2)|$ . The magnitude of the velocity,  $|E/k|$ , is given by  $v \cos(\phi/2)$ . We may also consider the direction of the spin for the wave functions in Eq. (24) with  $\gamma$  given by Eq. (27). We find that the spin points along the direction  $\hat{n} = \cos(\phi/2) \hat{y} - \sin(\phi/2) \hat{z}$  if  $k\phi > 0$  and along  $-\hat{n} = -\cos(\phi/2) \hat{y} + \sin(\phi/2) \hat{z}$  if  $k\phi < 0$ . It is interesting to note that  $\hat{n}$  lies half-way between  $\hat{y}$  and  $\hat{y}' = \cos \phi \hat{y} - \sin \phi \hat{z}$ .

## IV. JUNCTION BETWEEN SURFACE VELOCITIES WITH OPPOSITE SIGNS

Let us now study the case where there are two regions as in Sec. II, but the velocities  $v_1$  and  $v_2$  in those two regions have opposite signs<sup>28</sup>. To be specific, let us assume that  $v_1 > 0$  and  $v_2 < 0$ , and we send in a wave from region 1 with positive energy as before. Let us consider normal incidence, so that  $k_{Ix} = k_{Rx} = k_{Tx} = 0$ . We then see that the operator  $\sigma^x$  commutes with both  $H_1$  and  $H_2$ . For  $k_{Iy} > 0$  and positive energy  $E = v_1 k_{Iy}$ , the incident wave function is an eigenstate of  $\sigma^x$  with eigenvalue 1; hence the reflected and transmitted waves must also be eigenstates of  $\sigma^x$  with eigenvalue 1. However, this implies that the reflected wave must have  $k_{Ry} = k_{Iy}$  and the transmitted wave must have  $k_{Ty} = (v_1/v_2)k_{Iy}$ ; neither of this is possible since a reflected wave must have  $k_{Ry} < 0$  and a transmitted wave must have  $k_{Ty} > 0$ . We therefore see that the reflected and transmitted amplitudes must both vanish, leading to a difficulty in conserving the probability.



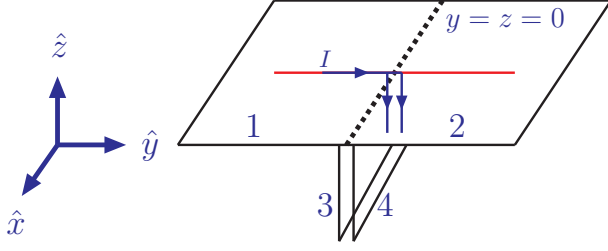


FIG. 6: (Color online) Schematic picture of two regions of the  $x - y$  plane, labeled 1 and 2, separated by a line junction at  $y = z = 0$ , and two additional surfaces, labeled 3 and 4, which lie in the  $x - z$  plane and are at the interface of the two TIs. A wave incident ( $I$ ) from region 1 at  $\theta = 0$  and transmitted waves in regions 3 and 4 are shown.

One way out of this difficulty is to look for a linear relation between  $(\psi_1)_{y \rightarrow 0-}$  and  $(\psi_2)_{y \rightarrow 0+}$  which satisfies current conservation as in Eq. (7). We find that the relation

$$(\psi_2)_{y \rightarrow 0+} = \sqrt{\frac{v_1}{|v_2|}} e^{-i\alpha\sigma^x} \sigma^z (\psi_1)_{y \rightarrow 0-} \quad (28)$$

works. However, there does not seem to be a physical way of justifying the factor of  $\sigma^z$  on the right hand side of Eq. (28), although the factor of  $e^{-i\alpha\sigma^x}$  can be justified in the same way as we did in the Appendix for the case of velocities with the same sign. In fact, the factor of  $\sigma^z$  in Eq. (28) makes it non-invariant under the transformation  $\psi_{1,2} \rightarrow \sigma^x \psi_{1,2}$  which was used above to show that the reflection and transmission amplitudes must vanish for normal incidence. The factor of  $\sigma^z$  would also break invariance under time reversal.

An alternative and physically appealing way out of the difficulty in conserving probability was proposed in Ref. 28, by realizing that in the case of opposite velocities, the waves must transmit *into* the interface regions 3 and 4 separating the two TIs, as depicted in Fig. 6. Regions 3 and 1 will both be taken to be surfaces of the first TI; we therefore assume that the velocity in both these regions is equal to  $v_1$ . Similarly, regions 4 and 2 are both surfaces of the second TI and therefore have the same velocity  $v_2$ . The line junction is therefore a boundary of four surfaces, namely, 1, 2, 3 and 4; the location of the line junction is given by  $y = 0$  for surfaces 1 and 2, and  $z = 0$  for surfaces 3 and 4 (with  $z$  becoming negative as one moves away from the line junction on these two surfaces). As we will discuss below, it will be convenient to assume that the line junction has a small width separating the first and second TIs. To see how a wave incident from region 1 can transmit into regions 3 and 4, we must first show that the interfaces 3 and 4 must necessarily have gapless states; otherwise energy conservation would not allow a very low-energy incident wave in region 1 to transmit into the interfaces 3 and 4. Let us therefore consider the Hamiltonian describing an electron moving on surfaces

3 and 4. Since 3 and 4 both lie in the  $x - z$  plane, but the unit vectors normal to those surfaces point in the  $\hat{y}$  and  $-\hat{y}$  directions respectively, the corresponding Hamiltonians are given by

$$\begin{aligned} H_3 &= -iv_1 (\sigma^z \partial_x - \sigma^x \partial_z), \\ H_4 &= iv_2 (\sigma^z \partial_x - \sigma^x \partial_z). \end{aligned} \quad (29)$$

Next, we examine what boundary condition must be imposed at the line junction so that the complete Hamiltonian is Hermitian. Since the system consists of four Hamiltonians,  $H_1$ ,  $H_2$ ,  $H_3$  and  $H_4$ , the general boundary condition which ensures Hermiticity will be much more involved than the one discussed in the Appendix for the case of two Hamiltonians. We will therefore consider the simplest possible boundary condition. Let us suppose that in the region of the line junction, the first TI (with surfaces 1 and 3) is separated from the second TI (with surfaces 2 and 4) by some distance; hence  $\psi_3$  will be connected to only  $\psi_1$ , and  $\psi_4$  will be connected to only  $\psi_2$ . Let us further assume that there is no potential barrier between surfaces 1 and 3 and between surfaces 2 and 4, so that the parameter  $\alpha$  introduced in Sec. II is now equal to zero. We then obtain the simple conditions

$$\psi_3 = \psi_1 \text{ and } \psi_4 = \psi_2 \quad (30)$$

at the line junction. (Note that this gives four equations since the  $\psi_i$  are all two-component spinors). This condition automatically implies that the incoming and outgoing currents normal to the line junction are equal to each other, namely,

$$v_1 \psi_1^\dagger \sigma^x \psi_1 - v_2 \psi_2^\dagger \sigma^x \psi_2 = v_1 \psi_3^\dagger \sigma^x \psi_3 - v_2 \psi_4^\dagger \sigma^x \psi_4. \quad (31)$$

Finally, we introduce tunneling between surfaces 3 and 4. Assuming rotational invariance in the  $x - z$  plane, the equations of motion take the form<sup>28</sup>

$$\begin{aligned} i\partial_t \psi_3 &= -iv_1 (\sigma^z \partial_x - \sigma^x \partial_z) \psi_3 + g \psi_4, \\ i\partial_t \psi_4 &= iv_2 (\sigma^z \partial_x - \sigma^x \partial_z) \psi_4 + g \psi_3, \end{aligned} \quad (32)$$

where  $g$  denotes the tunneling amplitude; we will assume that  $g$  is real and positive. In defining our model, we have made the conceptually simple assumption that the region of the line junction is distinct from the tunneling region so that the tunneling does not modify the boundary condition introduced in Eq. (30). (We note that the system described in Eq. (32) is invariant under the parity and time reversal transformations defined in Sec. II).

To make further analytical progress, let us assume that  $v_2 = -v_1$ . To find the energy spectrum and wave functions, we take

$$\psi_3 = u_3 e^{i(k_x x + k_z z - Et)}, \text{ and } \psi_4 = u_4 e^{i(k_x x + k_z z - Et)}, \quad (33)$$

where  $E > 0$  and  $u_3$  and  $u_4$  are two-component spinors. If  $u_3$ ,  $u_4$  are eigenstates of the operator  $\sigma^z k_x - \sigma^x k_z$  with eigenvalue  $k = \sqrt{k_x^2 + k_z^2}$ , the energy spectrum is

given by  $E = v_1 k \pm g$ , while if  $u_3, u_4$  are eigenstates of the same operator with eigenvalue  $-k$ , the energies are given by  $E = -v_1 k \pm g$ . We thus see that the energy vanishes, not at the origin  $(k_x, k_z) = (0, 0)$ , but on the circle  $\sqrt{k_x^2 + k_z^2} = g/v_1$ . This circle of points, along with  $E = 0$ , is not invariant under Lorentz transformations which will be discussed at the end of this section. Note that if  $v_2$  had been positive and equal to  $v_1$ , the energy spectrum of Eq. (32) would have taken a Lorentz invariant form as discussed below.

We now consider a wave incident on the line junction from region 1. Then there are four possibilities; it can get reflected back to region 1 with amplitude  $r$ , transmitted to region 2 with amplitude  $t$ , and transmitted to regions 3 and 4 with amplitudes  $t'$  and  $t''$  respectively. Since there are four amplitudes to be found and four matching conditions in Eq. (30), the scattering problem can be solved. In general, all the four amplitudes will be non-zero. However, let us now consider the case of normal incidence; then we indeed find that  $r = t = 0$  as expected due to the conservation of  $\sigma^x$ . To be explicit, the incident wave here is of the form

$$\psi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{i(ky - Et)}, \quad (34)$$

where  $E = v_1 k$ . Conservation of energy equal to  $E$ , momentum along the  $\hat{x}$  direction equal to zero, and  $\sigma^x$  equal to 1 in all the regions imply that the transmitted waves in regions 3 and 4 must be of the form

$$\begin{aligned} \psi_3 &= \frac{1}{2} \left[ t' \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ik'z} + t'' \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ik''z} \right] e^{-iEt}, \\ \psi_4 &= \frac{1}{2} \left[ t' \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ik'z} - t'' \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ik''z} \right] e^{-iEt}, \end{aligned} \quad (35)$$

where  $k' = (E/v_1) - g$  and  $k'' = (E/v_1) + g$ , and we have normalized the eigenstates corresponding to  $k'$  and  $k''$  to unity. The expressions in Eq. (35) are obtained by finding solutions of Eq. (32) with energy  $E$  and positive group velocities  $dE/dk'$  and  $dE/dk''$  so that they propagate in the  $-\hat{z}$  direction away from the line junction. Using Eq. (30) along with Eqs. (34-35) gives  $t' = t'' = 1/\sqrt{2}$ . Note that  $|r|^2 + |t|^2 + |t'|^2 + |t''|^2 = 1$  as desired.

The case of a general angle of incidence can be studied in a similar way. We assume that the plane waves associated with the incident wave in region 1 with amplitude 1, the reflected wave in region 1 with amplitude  $r$ , the transmitted wave in region 2 with amplitude  $t$ , and transmitted waves in regions 3 and 4 with amplitudes  $t'$  and  $t''$  are given by  $e^{i(k_x x + k_y y - Et)}$ ,  $e^{i(k_x x - k_y y - Et)}$ ,  $e^{i(k_x x + k_y y - Et)}$ ,  $e^{i(k_x x - k' z - Et)}$  and  $e^{i(k_x x - k'' z - Et)}$  respectively, where  $k_y > 0$ ,  $E = v_1 \sqrt{k_x^2 + k_y^2}$ ,  $k' = -\sqrt{(g - E/v_1)^2 - k_x^2}$ ,  $k'' = \sqrt{(g + E/v_1)^2 - k_x^2}$ , and we have assumed that  $0 < E/v_1 < g$  and  $g \pm E/v_1 > |k_x|$ . The above expressions and conditions ensure that the group velocity of the incident wave points toward the line junction but the

group velocities of the other four waves point away from the line junction as desired. We will not write down the corresponding two-component wave functions here, but simply note that the boundary conditions in Eq. (30) will provide four equations which will determine the values of  $r, t, t'$  and  $t''$ . In general, all these four amplitudes will be non-zero. In the limit that the angle of incidence  $\theta \rightarrow \pm\pi/2$ , we find that  $r \rightarrow -1$  and  $t, t', t'' \rightarrow 0$ .

We may return to the case of surface velocities with the same sign as discussed in Sec. II, and ask how the results for scattering from the line junction would change in that system if one introduces additional surfaces 3 and 4 coupled by a tunneling amplitude as in Fig. 6. Considering Eq. (32) with  $v_2 = v_1$ , we find that a tunneling amplitude  $g$  gives rise to an energy gap, instead of producing gapless states as in the case of velocities with opposite signs. To be specific, the energy spectrum of Eq. (32) would be given by  $E^2 = v_1^2(k_x^2 + k_z^2) + g^2$ , so that  $|E|$  has a minimum value of  $g$ . (Note that this form remains invariant under Lorentz transformations based on the velocity  $v_1$ . For instance,  $E^2 - v_1^2(k_x^2 + k_z^2)$  remains invariant under the transformation  $k_x \rightarrow (k_x - vE/v_1^2)/\sqrt{1 - v^2/v_1^2}$ ,  $E \rightarrow (E - vk_x)/\sqrt{1 - v^2/v_1^2}$  and  $k_z \rightarrow k_z$ , for any value of  $v$  whose magnitude is smaller than  $v_1$ ). As a result, an electron which is incident from region 1 with an energy less than  $g$  will either reflect back to region 1 or transmit to region 2, and the surfaces 3 and 4 will not play a role in this scattering problem.

## V. DISCUSSION

To summarize, we have shown that a number of interesting phenomena can occur at a line junction separating two surfaces of topological insulators. Assuming invariance under time reversal, a line junction can have an arbitrary parameter which makes the Hamiltonian Hermitian and is consistent with current conservation; this parameter may be understood as arising from a potential barrier lying along the junction. The conductance through the line junction depends on this parameter, and there may also be edge states which propagate along the junction. For a junction which separates two surfaces which are at an angle with respect to each other, we have shown that the conductance depends on the bending angle, and there are also edge states which lie along the junction. Our analysis has been based on simple models in which the junction width  $d$  has been taken to be zero; as a result, many properties of the edge states, such as their velocity and spin orientation, depend only on dimensionless parameters such as  $\alpha$  and  $\phi$  but not on the magnitude of the momentum  $k$  along the edge. Realistic junctions would have a finite width; the effects of the width need to be studied.

The edge states which lie along the junction differ in two ways from the plane wave states which lie far from the junction. The velocity of the edge states is always less than the velocities of the plane waves, so that the



energy of the edge states is smaller in magnitude from the energy of the plane waves for a given value of the momentum along the line junction. Secondly, the orientation of the spin of the edge states is generally different from the orientation of the plane waves; in particular, the spins of the edge states have a non-zero component in the direction perpendicular to the surfaces. These differences in the energy-momentum dispersion and the spin structure imply that it may be possible to observe various features of the edge states and to distinguish them from the plane waves (which reside far away from the line junction) by using spin-resolved angle-resolved photoemission spectroscopy and tunneling from a spin polarized STM tip placed close to the junction.

Finally, for the case in which the velocities on the two surfaces have opposite signs, we have explicitly demonstrated that a wave incident on the junction from either side must generally transmit into some additional surfaces which must emerge from the junction.

Before ending, we would like to point out that our analysis has ignored the effects of the hexagonal warping of the dispersion which is known to occur in TIs<sup>32</sup>. It would be interesting to study the effects of warping on the conductance through the junction and on the edge states. We would also like to mention recent studies of scattering and bound states near ferromagnetic domain walls on the surface of a TI<sup>33</sup>, transport across step junctions on a TI surface<sup>34,35</sup>, edge states induced by a magnetic field at junctions of two TI surfaces<sup>36</sup>, bulk models for studying states at surfaces with arbitrary orientations<sup>37</sup>, and tachyon-like states at the interface of two TIs<sup>38</sup>.

### Acknowledgments

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### Appendix A: General boundary condition which ensures Hermiticity

In this Appendix, we will discuss the general linear condition between  $(\chi_1)_{y \rightarrow 0^-}$  and  $(\chi_2)_{y \rightarrow 0^+}$  (and similarly for  $(\chi'_1)_{y \rightarrow 0^-}$  and  $(\chi'_2)_{y \rightarrow 0^+}$ ) which satisfies Eq. (3). Let us assume that

$$\begin{aligned} (\chi_2)_{y \rightarrow 0^+} &= U (\chi_1)_{y \rightarrow 0^-}, \\ (\chi'_2)_{y \rightarrow 0^+} &= U (\chi'_1)_{y \rightarrow 0^-}, \end{aligned} \quad (\text{A1})$$

where  $U$  is an arbitrary  $2 \times 2$  matrix. Then Eq. (3) will be satisfied if

$$U^\dagger \sigma^x U = \sigma^x. \quad (\text{A2})$$

Using the fact that the identity matrix  $I$  and the three Pauli matrices  $\vec{\sigma}$  form a basis for  $2 \times 2$  matrices, we find that the general solution to Eq. (A2) is given by

$$U = \exp[-i\alpha\sigma^x - i\beta - \gamma\sigma^y - \delta\sigma^z], \quad (\text{A3})$$

where  $\alpha$ ,  $\beta$ ,  $\gamma$  and  $\delta$  are real parameters; Eq. (A2) follows from the fact that  $U^\dagger \sigma^x = \sigma^x U^{-1}$ . (Eq. (A3) may be contrasted with the form of a unitary matrix  $V$  which satisfies  $V^\dagger V = I$ ; such a matrix can be written in terms of four real parameters as  $V = \exp[-i\alpha\sigma^x - i\beta - i\gamma\sigma^y - i\delta\sigma^z]$ ).

We will now present a model of a junction which provides a physical understanding of the four parameters appearing in Eq. (A3). Consider a thin barrier of width  $d$  extending from  $y = 0$  to  $y = d$  where there is a constant term  $V$  consisting of both potential and magnetic parts,

$$V(y) = A + B\sigma^x + C\sigma^z + D\sigma^y, \quad (\text{A4})$$

where  $A$ ,  $B$ ,  $C$  and  $D$  are real so that the Hamiltonian is Hermitian. We can think of  $A$  as a potential, and  $B$ ,  $C$  and  $D$  as being proportional to the three components of a magnetic field which has a Zeeman coupling to the spin of the electron. We will eventually be interested in the limit of a  $\delta$ -function barrier, so that  $A$ ,  $B$ ,  $C$ ,  $D \rightarrow \infty$  and  $d \rightarrow 0$  keeping  $Ad$ ,  $Bd$ ,  $Cd$  and  $Dd$  fixed.

The Hamiltonian in the region  $0 < y < d$  is now given by

$$H_d = -iv_2(\sigma^x \partial_y - \sigma^y \partial_x) + A + B\sigma^x + C\sigma^z + D\sigma^y. \quad (\text{A5})$$

Let us look for a state with energy  $E$  and momentum  $k$  in the  $\hat{x}$  direction; the corresponding wave function is of the form

$$\psi(x, y, t) = f(y) e^{i(kx - Et)}. \quad (\text{A6})$$

In the region  $0 < y < d$ ,  $f(y)$  satisfies the equation

$$\begin{aligned} [-iv_2 \sigma^x \partial_y - v_2 k \sigma^y + A + B\sigma^x + C\sigma^z + D\sigma^y] f \\ = Ef. \end{aligned} \quad (\text{A7})$$

Since we are interested in the limit  $A$ ,  $B$ ,  $C$ ,  $D \rightarrow \infty$ , we can ignore in Eq. (A7) the terms of order  $E$  and  $k$  which are finite. The solution for  $f$  is then given by

$$f(y) = \exp[(y/v_2)(-iA\sigma^x - iB - C\sigma^y + D\sigma^z)] f(0), \quad (\text{A8})$$

which implies that

$$f(d) = \exp[(d/v_2)(-iA\sigma^x - iB - C\sigma^y + D\sigma^z)] f(0). \quad (\text{A9})$$

We now take the limit  $A$ ,  $B$ ,  $C$ ,  $D \rightarrow \infty$  and  $d \rightarrow 0$  keeping  $Ad \equiv v_2\alpha$ ,  $Bd \equiv v_2\beta$ ,  $Cd \equiv v_2\gamma$  and  $Dd \equiv -v_2\delta$  fixed. By superposing states with different values of  $E$  and  $k$ , we then see that any wave function  $\psi(x, y, t)$  must satisfy

$$\psi(x, 0+, t) = \exp[-i\alpha\sigma^x - i\beta - \gamma\sigma^y - \delta\sigma^z] \psi(x, 0-, t). \quad (\text{A10})$$

This is the general boundary condition proposed in Eqs. (A1) and (A3).

Let us now impose invariance under time reversal. We then expect that only the potential  $A$  can remain non-zero in Eq. (A5) while the other three terms must be zero since they can be interpreted as arising from a magnetic field. To see this formally, we observe that under time reversal, we have to complex conjugate the Hamiltonians in Eq. (1) and wave functions, and transform the time  $t \rightarrow -t$ ; in addition, we have to do a unitary transformation by  $\sigma^y$  in order to maintain the form of the Hamiltonian. In other words,  $i\partial_t\psi = H\psi$  goes to  $i\partial_t\sigma^y\psi^* = \sigma^y H^* \sigma^y \psi^*$ , where  $\sigma^y H^* \sigma^y = H$ . On applying this transformation to Eq. (A5), we see that  $A$  can be non-zero but  $B$ ,  $C$  and  $D$  must vanish if  $V$  has to be time reversal invariant. Hence the parameters  $\beta$ ,  $\gamma$  and  $\delta$  must vanish in Eq. (A10). We are therefore left with the single parameter  $\alpha$  given in Eq. (4).

If  $\alpha \neq 0$ , the wave functions satisfying Eq. (4) are discontinuous at  $y = 0$  even if  $v_2 = v_1$ . This is not surprising. We recall that for the Schrödinger equation which is second order in spatial derivatives, a  $\delta$ -function potential barrier leads to a discontinuity in the first derivative of the wave function. For the Dirac equation which is first order in spatial derivative, a  $\delta$ -function potential leads to

a discontinuity in the wave function.

We would like to emphasize here that our aim has been to obtain the most general boundary condition consistent with certain Hamiltonians separated by a line junction. By doing so, we have included the effects of a thin barrier which could possibly be present at the junction. In a particular system of interest, the relevant parameters defining the boundary conditions would have to be determined from either the microscopic parameters of the system or from experimental studies of either transport across the junction or the edge states present there. For a given system (for instance, if there is actually no junction present so that the junction width  $d$  is exactly zero), it may turn out that all the four boundary parameters are equal to zero; however, this would only be a special case of our analysis.

To conclude, our analysis shows that in general four real parameters are required to completely specify the boundary condition; this generalizes the discussion in Refs. 28–31 where no such parameters were considered. A similar situation is known to arise for the Schrödinger equation with a discontinuity at one point; the general boundary condition at that point which ensures Hermiticity and conserves the current also has four parameters as discussed in Refs. 39 and 40.

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